

Unitary equivalent classes of one-dimensional quantum walks II

Hiromichi Ohno

Department of Mathematics, Faculty of Engineering, Shinshu University,
4-17-1 Wakasato, Nagano 380-8553, Japan

Abstract

This study investigated the unitary equivalent classes of one-dimensional quantum walks. We determined the unitary equivalent classes of one-dimensional quantum walks, two-phase quantum walks with one defect, complete two-phase quantum walks, one-dimensional quantum walks with one defect and translation-invariant one-dimensional quantum walks. The unitary equivalent classes of one-dimensional quantum walks with initial states were also considered.

1 Introduction

This study investigated the unitary equivalent classes of one-dimensional quantum walks. A quantum walk is defined by a pair $(U, \{\mathcal{H}_v\}_{v \in V})$, in which V is a countable set, $\{\mathcal{H}_v\}_{v \in V}$ is a family of separable Hilbert spaces, and U is a unitary operator on $\mathcal{H} = \bigoplus_{v \in V} \mathcal{H}_v$ [20]. In this paper, we discuss one-dimensional (two-state) quantum walks, in which $V = \mathbb{Z}$ and $\mathcal{H}_v = \mathbb{C}^2$. These have been the subject of many previous studies [1, 2, 4, 6–19, 21–23].

It is important to clarify what it means to say that two quantum walks are the same. We define unitary equivalence in the same way as [19, 20]. If two quantum walks are unitary equivalent, then their digraphs, dimensions of their Hilbert spaces, and the probability distributions of the quantum walks are the same.

In the previous paper [19], we discussed some general properties of unitary equivalent quantum walks. In particular, we proved that every one-dimensional quantum walk is the unitary equivalent of one of the Ambainis type. We also presented the necessary and sufficient condition for defining a one-dimensional quantum walk as a Szegedy walk.

Unitary equivalent classes of simple quantum walks have been shown to be parameterized by a single parameter [12]. In contrast, there are several types of one-dimensional quantum walks, including two-phase quantum walks with one defect [6, 7], complete two-phase quantum walks [11], and one-dimensional quantum walks with one defect [4, 8–10, 17, 18, 23]. In this study, we clarified the unitary equivalent classes of general one-dimensional quantum walks and of the above types of one-dimensional quantum walk, but excluding certain special cases. In Sect. 2, we present our results: two-phase quantum walks with one defect are parameterized by six parameters, complete two-phase quantum walks by four parameters, and one-dimensional quantum walks with one defect by four parameters.

When studying the probability distribution of a quantum walk, an initial state must be set and a quantum walk with an initial state must also be considered. In Sect. 3, we present

unitary equivalent classes of all the above types of one-dimensional quantum walk with an initial state.

2 Unitary equivalent classes of one-dimensional quantum walks

We first consider the definition of a one-dimensional quantum walk and the unitary equivalence of such walks (see [19]).

Definition 2.1 Let $\mathcal{H}_n = \mathbb{C}^2$ for $n \in \mathbb{Z}$. A unitary operator U on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$ is called a one-dimensional quantum walk if

$$\text{rank } P_n U P_m = \begin{cases} 1 & (m = n \pm 1) \\ 0 & (m \neq n \pm 1) \end{cases}$$

for all $m, n \in \mathbb{Z}$, where P_n is the projection onto \mathcal{H}_n .

A (pure) quantum state is represented by a unit vector in a Hilbert space. For $\lambda \in \mathbb{R}$, quantum states ξ and $e^{i\lambda}\xi$ in \mathcal{H} are identified. Hence, the one-dimensional quantum walks U and $e^{i\lambda}U$ are also identified.

Definition 2.2 One-dimensional quantum walks U_1 and U_2 are unitary equivalent if there exists a unitary $W = \bigoplus_{n \in \mathbb{Z}} W_n$ on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$ such that

$$W U_1 W^* = U_2.$$

Theorem 1 in [19] (see also the first paragraph of Section 5 in [19]) yields the next theorem.

Theorem 2.3 A one-dimensional quantum walk U is described as follows:

$$U = \sum_{n \in \mathbb{Z}} |\xi_{n-1,n}\rangle \langle \zeta_{n-1,n}| + |\xi_{n+1,n}\rangle \langle \zeta_{n+1,n}|, \quad (1)$$

where $\{\xi_{n,n+1}, \xi_{n+1,n}\}_{n \in \mathbb{Z}}$ and $\{\zeta_{n,n+1}, \zeta_{n+1,n}\}_{n \in \mathbb{Z}}$ are orthonormal bases of $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$ with $\xi_{n,n+1}, \zeta_{n+1,n} \in \mathcal{H}_n$ and $\xi_{n+1,n}, \zeta_{n,n+1} \in \mathcal{H}_{n+1}$.

The unitary equivalence of a one-dimensional quantum walk can then be analyzed as follows.

Step 1. Assume that U is described as in (1), and define a unitary operator W_1 on \mathcal{H} as

$$W_1 = \bigoplus_{n \in \mathbb{Z}} |e_1^n\rangle \langle \xi_{n,n+1}| + |e_2^n\rangle \langle \xi_{n,n-1}|,$$

where $\{e_1^n, e_2^n\}$ is the standard basis of $\mathcal{H}_n = \mathbb{C}^2$. Then,

$$\begin{aligned} W_1 U W_1^* &= \sum_{n \in \mathbb{Z}} |W_1 \xi_{n-1,n}\rangle \langle W_1 \zeta_{n-1,n}| + |W_1 \xi_{n+1,n}\rangle \langle W_1 \zeta_{n+1,n}| \\ &= \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle e^{ia_n} r_n e_1^n + e^{ib_n} s_n e_2^n| + |e_2^{n+1}\rangle \langle e^{ic_n} s_n e_1^n + e^{id_n} r_n e_2^n| \end{aligned} \quad (2)$$

for some $0 \leq r_n \leq 1$ and $a_n, b_n, c_n, d_n \in \mathbb{R}$ with $s_n = \sqrt{1 - r_n^2}$ and

$$a_n - b_n = c_n - d_n + \pi \pmod{2\pi}. \quad (3)$$

If there is no confusion, $\pmod{2\pi}$ can be omitted hereafter.

Step 2. Define $g_n \in \mathbb{R}$ by $g_0 = 0$ and

$$g_{n-1} - g_n = a_n,$$

inductively. Similarly, define $h_n \in \mathbb{R}$ by $h_0 = g_{-1} - b_0$ and

$$h_{n+1} - h_n = d_n,$$

inductively. Then, by (3),

$$c_n - h_{n+1} + g_n = c_n - h_n - d_n + g_{n-1} - a_n = -(b_n - g_{n-1} + h_n) + \pi \pmod{2\pi}. \quad (4)$$

Let W_2 be a unitary operator defined by

$$W_2 = \bigoplus_{n \in \mathbb{Z}} e^{ig_n} |e_1^n\rangle \langle e_1^n| + e^{ih_n} |e_2^n\rangle \langle e_2^n|.$$

By definitions and (4),

$$\begin{aligned} & W_2 W_1 U W_1^* W_2^* \\ &= \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle e^{i(a_n - g_{n-1} + g_n)} r_n e_1^n + e^{i(b_n - g_{n-1} + h_n)} s_n e_2^n| \\ & \quad + |e_2^{n+1}\rangle \langle e^{i(c_n - h_{n+1} + g_n)} s_n e_1^n + e^{i(d_n - h_{n+1} + h_n)} r_n e_2^n| \\ &= \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle r_n e_1^n + e^{ik_n} s_n e_2^n| + |e_2^{n+1}\rangle \langle -e^{-ik_n} s_n e_1^n + r_n e_2^n|, \end{aligned}$$

where $k_n = b_n - g_{n-1} + h_n$. Here,

$$k_0 = b_0 - g_{-1} + h_0 = 0.$$

Step 3. Let $\ell = k_1/2$, $p_n = nk_1/2$ and $q_n = -nk_1/2$, and let

$$W_3 = \bigoplus_{n \in \mathbb{Z}} e^{ip_n} |e_1^n\rangle \langle e_1^n| + e^{iq_n} |e_2^n\rangle \langle e_2^n|.$$

Then,

$$\begin{aligned} & e^{i\ell} W_3 W_2 W_1 U W_1^* W_2^* W_3^* \\ &= \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle e^{i(-p_{n-1} + p_n - \ell)} r_n e_1^n + e^{i(k_n - p_{n-1} + q_n - \ell)} s_n e_2^n| \\ & \quad + |e_2^{n+1}\rangle \langle -e^{i(-k_n - q_{n+1} + p_n - \ell)} s_n e_1^n + e^{i(-q_{n+1} + q_n - \ell)} r_n e_2^n| \\ &= \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle r_n e_1^n + e^{i(k_n - nk_1)} s_n e_2^n| + |e_2^{n+1}\rangle \langle -e^{i(-k_n + nk_1)} s_n e_1^n + r_n e_2^n| \\ &= \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle r_n e_1^n + e^{i\theta_n} s_n e_2^n| + |e_2^{n+1}\rangle \langle -e^{-i\theta_n} s_n e_1^n + r_n e_2^n|, \end{aligned}$$

where $\theta_n = k_n - nk_1$. Here, $\theta_0 = \theta_1 = 0$.

Consequently, we have the next theorem.

Theorem 2.4 *A one-dimensional quantum walk U is unitary equivalent to*

$$U_{r,\theta} = \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle r_n e_1^n + e^{i\theta_n} s_n e_2^n| + |e_2^{n+1}\rangle \langle -e^{-i\theta_n} s_n e_1^n + r_n e_2^n|$$

for some $0 \leq r_n \leq 1$ and $\theta_n \in \mathbb{R}$ with $s_n = \sqrt{1 - r_n^2}$ and $\theta_0 = \theta_1 = 0$.

The operator $U_{r,\theta}$ is similar to the CMV matrix introduced in [3, 5]. However, our approach and result are different in three ways from those used in [3, 5]. First, our starting point is the general one-dimensional quantum walk. Second, we add the condition $\theta_0 = \theta_1 = 0$. Third, with the exception of certain special cases, $U_{r,\theta}$ and $U_{r',\theta'}$ are not unitary equivalent if $r \neq r'$ or $\theta \neq \theta'$, as can be seen from the next theorem.

Theorem 2.5 *When $0 < r_n, r'_n < 1$ and $\theta_n, \theta'_n \in [0, 2\pi)$, $U_{r,\theta}$ and $U_{r',\theta'}$ are unitary equivalent if and only if $r = r'$ and $\theta = \theta'$.*

Proof. We assume that $U_{r,\theta}$ and $U_{r',\theta'}$ are unitary equivalent, where $0 < r_n, r'_n < 1$ and $\theta_n, \theta'_n \in [0, 2\pi)$ with $\theta_0 = \theta_1 = \theta'_0 = \theta'_1 = 0$. Then, there exist $\lambda \in \mathbb{R}$ and a unitary operator $W = \bigoplus_{n \in \mathbb{Z}} W_n$ on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$ such that

$$e^{i\lambda} W U_{r,\theta} W^* = U_{r',\theta'}.$$

Then,

$$e^{i\lambda} W U_{r,\theta} W^* = e^{i\lambda} \sum_{n \in \mathbb{Z}} |W e_1^{n-1}\rangle \langle r_n W e_1^n + e^{i\theta_n} s_n W e_2^n| + |W e_2^{n+1}\rangle \langle -e^{-i\theta_n} s_n W e_1^n + r_n W e_2^n|$$

and

$$U_{r',\theta'} = \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle r'_n e_1^n + e^{i\theta'_n} s'_n e_2^n| + |e_2^{n+1}\rangle \langle -e^{-i\theta'_n} s'_n e_1^n + r'_n e_2^n|.$$

Since $P_{n \pm 1} e^{i\lambda} W U_{r,\theta} W^* P_n = P_{n \pm 1} U_{r',\theta'} P_n$ for all $n \in \mathbb{Z}$, $W e_1^n$ and $W e_2^n$ are described as $W e_1^n = e^{iu_n} e_1^n$ and $W e_2^n = e^{iv_n} e_2^n$ for some $u_n, v_n \in \mathbb{R}$. Then,

$$\begin{aligned} & e^{i\lambda} W U_{r,\theta} W^* \\ &= \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle \langle e^{i(-u_{n-1}+u_n-\lambda)} r_n e_1^n + e^{i(\theta_n-u_{n-1}+v_n-\lambda)} s_n e_2^n| \\ & \quad + |e_2^{n+1}\rangle \langle -e^{i(-\theta_n-v_{n+1}+u_n-\lambda)} s_n e_1^n + e^{i(-v_{n+1}+v_n-\lambda)} r_n e_2^n|. \end{aligned} \tag{5}$$

Comparing the coefficients of $|e_1^{n-1}\rangle \langle e_1^n|$ and $|e_2^{n+1}\rangle \langle e_2^n|$ yields

$$-u_{n-1} + u_n - \lambda = 0, \quad -v_{n+1} + v_n - \lambda = 0.$$

Here, we can assume that $u_0 = 0$ because $W U W^* = (e^{iw} W) U (e^{iw} W)^*$ for any $w \in \mathbb{R}$. Therefore, $u_n = n\lambda$. Moreover, the coefficients of $|e_1^{-1}\rangle \langle e_2^0|$ imply

$$0 = \theta'_0 = \theta_0 - u_{-1} + v_0 - \lambda$$

with the result that $v_0 = 0$. Hence, $v_n = -n\lambda$. Similarly, the coefficients of $|e_1^0\rangle \langle e_2^1|$ imply

$$0 = \theta'_1 = \theta_1 - u_0 + v_1 - \lambda = -2\lambda \pmod{2\pi}$$

with the result that $\lambda = 0, \pi$. When $\lambda = 0$, $u_n = v_n = 0$, and therefore, $W = I_{\mathcal{H}}$ and $U_{r,\theta} = U_{r',\theta'}$. When $\lambda = \pi$, $u_n = n\pi$ and $v_n = -n\pi = n\pi \pmod{2\pi}$. In this case, $W = \bigoplus_{n \in \mathbb{Z}} (-1)^n I_{\mathcal{H}_n}$. By (5), we have $e^{i\lambda} W U_{r,\theta} W^* = U_{r,\theta}$, and therefore, $U_{r,\theta} = U_{r',\theta'}$. It is easy to see that $U_{r,\theta} = U_{r',\theta'}$ implies that $r = r'$ and $\theta = \theta'$.

The converse is obvious. \square

We next consider some special cases of the one-dimensional quantum walk, and introduce four types of one-dimensional quantum walk.

Definition 2.6 *Let U be a one-dimensional quantum walk expressed by*

$$U = \sum_{n \in \mathbb{Z}} |\xi_{n-1,n}\rangle \langle \zeta_{n-1,n}| + |\xi_{n+1,n}\rangle \langle \zeta_{n+1,n}|.$$

(i) *U is called a translation-invariant quantum walk if there exist $\xi_1, \xi_2, \zeta_1, \zeta_2 \in \mathbb{C}^2$ such that*

$$\xi_{n,n+1} = \xi_1, \quad \xi_{n,n-1} = \xi_2, \quad \zeta_{n-1,n} = \zeta_1, \quad \zeta_{n+1,n} = \zeta_2$$

for all $n \in \mathbb{Z}$. In other words, the vectors $\xi_{n,n+1}$ are the same, and $\xi_{n,n-1}, \zeta_{n-1,n}, \zeta_{n+1,n}$ also satisfy similar conditions.

(ii) *U is called a one-dimensional quantum walk with one defect if there exist $\xi_1, \xi_2, \zeta_1, \zeta_2 \in \mathbb{C}^2$ such that*

$$\xi_{n,n+1} = \xi_1, \quad \xi_{n,n-1} = \xi_2, \quad \zeta_{n-1,n} = \zeta_1, \quad \zeta_{n+1,n} = \zeta_2$$

for all $n \in \mathbb{Z} \setminus \{0\}$. In other words, the vectors $\xi_{n,n+1}$ are the same except $n \neq 0$, and $\xi_{n,n-1}, \zeta_{n-1,n}, \zeta_{n+1,n}$ also satisfy similar conditions.

(iii) *U is called a complete two-phase quantum walk if there exist $\xi_1^+, \xi_1^-, \xi_2^+, \xi_2^-, \zeta_1^+, \zeta_1^-, \zeta_2^+, \zeta_2^- \in \mathbb{C}^2$ such that*

$$\xi_{n,n+1} = \xi_1^+, \quad \xi_{n,n-1} = \xi_2^+, \quad \zeta_{n-1,n} = \zeta_1^+, \quad \zeta_{n+1,n} = \zeta_2^+$$

for all $n \geq 0$ and

$$\xi_{n,n+1} = \xi_1^-, \quad \xi_{n,n-1} = \xi_2^-, \quad \zeta_{n-1,n} = \zeta_1^-, \quad \zeta_{n+1,n} = \zeta_2^-$$

for all $n \leq -1$.

(iv) *U is called a two-phase quantum walk with one defect if there exist $\xi_1^+, \xi_1^-, \xi_2^+, \xi_2^-, \zeta_1^+, \zeta_1^-, \zeta_2^+, \zeta_2^- \in \mathbb{C}^2$ such that*

$$\xi_{n,n+1} = \xi_1^+, \quad \xi_{n,n-1} = \xi_2^+, \quad \zeta_{n-1,n} = \zeta_1^+, \quad \zeta_{n+1,n} = \zeta_2^+ \tag{6}$$

for all $n \geq 1$ and

$$\xi_{n,n+1} = \xi_1^-, \quad \xi_{n,n-1} = \xi_2^-, \quad \zeta_{n-1,n} = \zeta_1^-, \quad \zeta_{n+1,n} = \zeta_2^- \tag{7}$$

for all $n \leq -1$.

The next theorem describes the unitary equivalent classes of two-phase quantum walks with one defect.

Theorem 2.7 *A two-phase quantum walk U with one defect is unitary equivalent to*

$$\begin{aligned} U_{r_+, r_-, r_0, \mu_1, \mu_2, \mu_3} &= |e_1^{-1}\rangle \langle r_0 e_1^0 + e^{i\mu_1} s_0 e_2^0| + |e_2^1\rangle \langle -e^{i\mu_2} s_0 e_1^0 + e^{i(\mu_1 + \mu_2)} r_0 e_2^0| \\ &+ \sum_{n \geq 1} |e_1^{n-1}\rangle \langle r_+ e_1^n + s_+ e_2^n| + |e_2^{n+1}\rangle \langle -e^{i\mu_3} s_+ e_1^n + e^{i\mu_3} r_+ e_2^n| \\ &+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle r_- e_1^n + s_- e_2^n| + |e_2^{n+1}\rangle \langle -s_- e_1^n + r_- e_2^n| \end{aligned}$$

for some $0 \leq r_+, r_-, r_0 \leq 1$ and $\mu_1, \mu_2, \mu_3 \in \mathbb{R}$ with $s_\varepsilon = \sqrt{1 - r_\varepsilon^2}$ ($\varepsilon = +, -, 0$). We write $U_{r_+, r_-, r_0, \mu_1, \mu_2, \mu_3} = U_{r, \mu}$ for short.

Proof. Let

$$U = \sum_{n \in \mathbb{Z}} |\xi_{n-1, n}\rangle \langle \zeta_{n-1, n}| + |\xi_{n+1, n}\rangle \langle \zeta_{n+1, n}|$$

be a two-phase quantum walk with one defect. Then, by (6) and (7), Equation (2) can be written as

$$\begin{aligned} W_1 U W_1^* &= |e_1^{-1}\rangle \langle e^{ia_0} r_0 e_1^0 + e^{ib_0} s_0 e_2^0| + |e_2^1\rangle \langle e^{ic_0} s_0 e_1^0 + e^{id_0} r_0 e_2^0| \\ &+ \sum_{n \geq 1} |e_1^{n-1}\rangle \langle e^{ia_+} r_+ e_1^n + e^{ib_+} s_+ e_2^n| + |e_2^{n+1}\rangle \langle e^{ic_+} s_+ e_1^n + e^{id_+} r_+ e_2^n| \\ &+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle e^{ia_-} r_- e_1^n + e^{ib_-} s_- e_2^n| + |e_2^{n+1}\rangle \langle e^{ic_-} s_- e_1^n + e^{id_-} r_- e_2^n| \end{aligned} \quad (8)$$

for some $0 \leq r_\varepsilon \leq 1$ and $a_\varepsilon, b_\varepsilon, c_\varepsilon, d_\varepsilon \in \mathbb{R}$ with $s_\varepsilon = \sqrt{1 - r_\varepsilon^2}$ ($\varepsilon = +, -, 0$).

We then modify Step 2 as follows:

Step 2'. Let $\ell = (b_- + c_- + \pi)/2$. Define $g_n, h_n \in \mathbb{R}$ by

$$g_n = \begin{cases} n(\ell - a_+) & (n \geq 0) \\ n(\ell - a_-) - a_- + a_0 & (n \leq -1) \end{cases}$$

and

$$h_n = \begin{cases} (n-1)(\ell - a_+) - b_+ + \ell & (n \geq 1) \\ (n-1)(\ell - a_-) + c_- + a_0 - a_- - \ell + \pi & (n \leq 0) \end{cases},$$

and a unitary W_2 on \mathcal{H} by

$$W_2 = \bigoplus_{n \in \mathbb{Z}} e^{ig_n} |e_1^n\rangle \langle e_1^n| + e^{ih_n} |e_2^n\rangle \langle e_2^n|.$$

Then, using $a_\varepsilon + d_\varepsilon + \pi = b_\varepsilon + c_\varepsilon$,

$$\begin{aligned}
& e^{i\ell} W_2 W_1 U W_1^* W_2^* \\
&= |e_1^{-1}\rangle \langle e^{i(a_0-g_{-1}+g_0-\ell)} r_0 e_1^0 + e^{i(b_0-g_{-1}+h_0-\ell)} s_0 e_2^0| \\
&\quad + |e_2^1\rangle \langle e^{i(c_0-h_1+g_0-\ell)} s_0 e_1^0 + e^{i(d_0-h_1+h_0-\ell)} r_0 e_2^0| \\
&+ \sum_{n \geq 1} |e_1^{n-1}\rangle \langle e^{i(a_+-g_{n-1}+g_n-\ell)} r_+ e_1^n + e^{i(b_+-g_{n-1}+h_n-\ell)} s_+ e_2^n| \\
&\quad + |e_2^{n+1}\rangle \langle e^{i(c_+-h_{n+1}+g_n-\ell)} s_+ e_1^n + e^{i(d_+-h_{n+1}+h_n-\ell)} r_+ e_2^n| \\
&+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle e^{i(a_--g_{n-1}+g_n-\ell)} r_- e_1^n + e^{i(b_--g_{n-1}+h_n-\ell)} s_- e_2^n| \\
&\quad + |e_2^{n+1}\rangle \langle e^{i(c_--h_{n+1}+g_n-\ell)} s_- e_1^n + e^{i(d_--h_{n+1}+h_n-\ell)} r_- e_2^n| \\
&= |e_1^{-1}\rangle \langle r_0 e_1^0 + e^{i(b_0-b_-)} s_0 e_2^0| + |e_2^1\rangle \langle -e^{i(b_+-b_-+c_0-c_-)} s_0 e_1^0 + e^{i(b_0+b_+-2b_-+c_0-c_-)} r_0 e_2^0| \\
&+ \sum_{n \geq 1} |e_1^{n-1}\rangle \langle r_+ e_1^n + s_+ e_2^n| + |e_2^{n+1}\rangle \langle -e^{i(b_+-b_-+c_+-c_-)} s_+ e_1^n + e^{i(b_+-b_-+c_+-c_-)} r_+ e_2^n| \\
&+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle r_- e_1^n + s_- e_2^n| + |e_2^{n+1}\rangle \langle -s_- e_1^n + r_- e_2^n| \\
&= |e_1^{-1}\rangle \langle r_0 e_1^0 + e^{i\mu_1} s_0 e_2^0| + |e_2^1\rangle \langle -e^{i\mu_2} s_0 e_1^0 + e^{i(\mu_1+\mu_2)} r_0 e_2^0| \\
&+ \sum_{n \geq 1} |e_1^{n-1}\rangle \langle r_+ e_1^n + s_+ e_2^n| + |e_2^{n+1}\rangle \langle -e^{i\mu_3} s_+ e_1^n + e^{i\mu_3} r_+ e_2^n| \\
&+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle r_- e_1^n + s_- e_2^n| + |e_2^{n+1}\rangle \langle -s_- e_1^n + r_- e_2^n| \\
&= U_{r,\mu},
\end{aligned}$$

where $\mu_1 = b_0 - b_-$, $\mu_2 = b_+ - b_- + c_0 - c_+$ and $\mu_3 = b_+ - b_- + c_+ - c_-$. \square

The next theorem considers unitary equivalence between $U_{r,\mu}$ and $U_{r',\mu'}$.

Theorem 2.8 *When $0 < r_\varepsilon, r'_\varepsilon < 1$ ($\varepsilon = +, -, 0$) and $\mu_i, \mu'_i \in [0, 2\pi)$ ($i = 1, 2, 3$), $U_{r,\mu}$ and $U_{r',\mu'}$ are unitary equivalent if and only if $r = r'$, $\mu = \mu'$.*

Proof. We assume that $U_{r,\mu}$ and $U_{r',\mu'}$ are unitary equivalent, where $0 < r_\varepsilon, r'_\varepsilon < 1$ and $\mu_i, \mu'_i \in [0, 2\pi)$. Then, there exist $\lambda \in \mathbb{R}$ and a unitary operator $W = \bigoplus_{n \in \mathbb{Z}} W_n$ on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$ such that

$$e^{i\lambda} W U_{r,\mu} W^* = U_{r',\mu'}.$$

Here,

$$\begin{aligned}
& e^{i\lambda} W U_{r,\mu} W^* \\
&= e^{i\lambda} |W e_1^{-1}\rangle \langle r_0 W e_1^0 + e^{i\mu_1} s_0 W e_2^0| + e^{i\lambda} |W e_2^1\rangle \langle -e^{i\mu_2} s_0 W e_1^0 + e^{i(\mu_1+\mu_2)} r_0 W e_2^0| \\
&+ e^{i\lambda} \sum_{n \geq 1} |W e_1^{n-1}\rangle \langle r_+ W e_1^n + s_+ W e_2^n| + |W e_2^{n+1}\rangle \langle -e^{i\mu_3} s_+ W e_1^n + e^{i\mu_3} r_+ W e_2^n| \\
&+ e^{i\lambda} \sum_{n \leq -1} |W e_1^{n-1}\rangle \langle r_- W e_1^n + s_- W e_2^n| + |W e_2^{n+1}\rangle \langle -s_- W e_1^n + r_- W e_2^n|
\end{aligned}$$

and

$$\begin{aligned}
U_{r',\mu'} &= |e_1^{-1}\rangle\langle r'_0 e_1^0 + e^{i\mu'_1} s'_0 e_2^0| + |e_2^1\rangle\langle -e^{i\mu'_2} s'_0 e_1^0 + e^{i(\mu'_1+\mu'_2)} r'_0 e_2^0| \\
&+ \sum_{n \geq 1} |e_1^{n-1}\rangle\langle r'_+ e_1^n + s'_+ e_2^n| + |e_2^{n+1}\rangle\langle -e^{i\mu'_3} s'_+ e_1^n + e^{i\mu'_3} r'_+ e_2^n| \\
&+ \sum_{n \leq -1} |e_1^{n-1}\rangle\langle r'_- e_1^n + s'_- e_2^n| + |e_2^{n+1}\rangle\langle -s'_- e_1^n + r'_- e_2^n|.
\end{aligned}$$

Considering $P_{n \pm 1} e^{i\lambda} W U_{r,\mu} W^* P_n = P_{n \pm 1} U_{r',\mu'} P_n$ for any $n \in \mathbb{Z}$, we have $W e_1^n = e^{iu_n} e_1^n$ and $W e_2^n = e^{iv_n} e_2^n$ for some $u_n, v_n \in \mathbb{R}$. Then,

$$\begin{aligned}
&e^{i\lambda} W U_{r,\mu} W^* \\
&= |e_1^{-1}\rangle\langle e^{i(-u_{-1}+u_0-\lambda)} r_0 e_1^0 + e^{i(-u_{-1}+v_0-\lambda+\mu_1)} s_0 e_2^0| \\
&\quad + |e_2^1\rangle\langle -e^{i(-v_1+u_0-\lambda+\mu_2)} s_0 e_1^0 + e^{i(-v_1+v_0-\lambda+\mu_1+\mu_2)} r_0 e_2^0| \\
&+ \sum_{n \geq 1} |e_1^{n-1}\rangle\langle e^{i(-u_{n-1}+u_n-\lambda)} r_+ e_1^n + e^{i(-u_{n-1}+v_n-\lambda)} s_+ e_2^n| \\
&\quad + |e_2^{n+1}\rangle\langle -e^{i(-v_{n+1}+u_n-\lambda+\mu_3)} s_+ e_1^n + e^{i(-v_{n+1}+v_n-\lambda+\mu_3)} r_+ e_2^n| \\
&+ \sum_{n \leq -1} |e_1^{n-1}\rangle\langle e^{i(-u_{n-1}+u_n-\lambda)} r_- e_1^n + e^{i(-u_{n-1}+v_n-\lambda)} s_- e_2^n| \\
&\quad + |e_2^{n+1}\rangle\langle -e^{i(-v_{n+1}+u_n-\lambda)} s_- e_1^n + e^{i(-v_{n+1}+v_n-\lambda)} r_- e_2^n|. \tag{9}
\end{aligned}$$

Since $e^{i\lambda} W U_{r,\mu} W^* = U_{r',\mu'}$, we obtain $r = r'$. Moreover, comparing the coefficients of $|e_1^{n-1}\rangle\langle e_1^n|$, $|e_1^{n-1}\rangle\langle e_2^n|$ and $|e_2^{n+1}\rangle\langle e_2^n|$ yields

$$-u_{n-1} + u_n - \lambda = 0, \quad -u_{n-1} + v_n - \lambda = 0 \ (n \neq 0), \quad -v_{n+1} + v_n - \lambda = 0 \ (n \leq -1). \tag{10}$$

Here, we can assume that $u_0 = 0$, because $W U W^* = (e^{iw} W) U (e^{iw} W)^*$ for any $w \in \mathbb{R}$. Therefore, $u_n = n\lambda$, and this implies $v_n = u_{n-1} + \lambda = n\lambda$ ($n \neq 0$). Using the third equation in (10), we have $2\lambda = 0$, and therefore $\lambda = 0$ or π . Moreover, the coefficients of $|e_2^0\rangle\langle e_1^{-1}|$ imply $v_0 = u_{-1} - \lambda = -2\lambda = 0$. Comparing the coefficients of $|e_1^{-1}\rangle\langle e_2^0|$, $|e_2^1\rangle\langle e_1^0|$ and $|e_2^{n+1}\rangle\langle e_2^n|$ ($n \geq 1$), we obtain $\mu = \mu'$. \square

From the above proof, if $e^{i\lambda} W U_{r,\mu} W^* = U_{r,\mu}$, then $\lambda = 0$ or π . When $\lambda = 0$, $v_n = u_n = 0$ and $W = I_{\mathcal{H}}$. When $\lambda = \pi$, $v_n = u_n = n\pi$ and $W = \bigoplus_{n \in \mathbb{Z}} (-1)^n I_{\mathcal{H}_n}$. Hence, we have the next corollary.

Corollary 2.9 *Let $0 < r_\varepsilon < 1$ ($\varepsilon = +, -, 0$) and $\mu_i \in [0, 2\pi)$, and let $W = \bigoplus_{n \in \mathbb{Z}} W_n$ be a unitary on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$. Then, for $\lambda \in [0, 2\pi)$,*

$$e^{i\lambda} W U_{r,\mu} W^* = U_{r,\mu}$$

if and only if $\lambda = 0$ and $W = I_{\mathcal{H}}$ or $\lambda = \pi$ and $W = \bigoplus_{n \in \mathbb{Z}} (-1)^n I_{\mathcal{H}_n}$.

As a corollary of Theorem 2.7 and 2.8, we obtain the following.

Corollary 2.10 [12] *A translation-invariant quantum walk U is unitary equivalent to*

$$U_r = \sum_{n \in \mathbb{Z}} |e_1^{n-1}\rangle\langle r e_1^n + s e_2^n| + |e_2^{n+1}\rangle\langle s e_1^n + r e_2^n|$$

for some $0 \leq r \leq 1$ with $s = \sqrt{1-r^2}$. Moreover, U_r and $U_{r'}$ are unitary equivalent if and only if $r = r'$.

Proof. From the definition of a translation-invariant quantum walk, we can assume that, in (8), $r_+ = r_- = r_0$, $a_+ = a_- = a_0$ and so on. This implies that $\mu_1 = b_0 - b_- = 0$, $\mu_2 = b_+ - b_- + c_0 - c_+ = 0$ and $\mu_3 = b_+ - b_- + c_+ - c_- = 0$. Setting $r = r_0$ satisfies the first assertion. The necessary and sufficient condition for unitary equivalence follows from Theorem 2.8. \square

Corollary 2.11 *A one-dimensional quantum walk U with one defect is unitary equivalent to*

$$U_{r_{\pm}, r_0, \nu_1, \nu_2} = |e_1^{-1}\rangle\langle r_0 e_1^0 + e^{i\nu_1} s_0 e_2^0| + |e_2^1\rangle\langle -e^{i\nu_2} s_0 e_1^0 + e^{i(\nu_1 + \nu_2)} r_0 e_2^0| \\ + \sum_{n \in \mathbb{Z} \setminus \{0\}} |e_1^{n-1}\rangle\langle r_{\pm} e_1^n + s_{\pm} e_2^n| + |e_2^{n+1}\rangle\langle s_{\pm} e_1^n + r_{\pm} e_2^n|$$

for some $0 \leq r_{\varepsilon} \leq 1$ and $\nu_1, \nu_2 \in \mathbb{R}$ with $s_{\varepsilon} = \sqrt{1 - r_{\varepsilon}^2}$ ($\varepsilon = \pm, 0$). We write $U_{r_{\pm}, r_0, \nu_1, \nu_2} = U_{r, \nu}$ for short. Moreover, when $0 < r_{\varepsilon}, r'_{\varepsilon} < 1$ and $\nu_i, \nu'_i \in [0, 2\pi)$, $U_{r, \nu}$ and $U_{r', \nu'}$ are unitary equivalent if and only if $r = r'$ and $\nu = \nu'$.

Proof. From the definition of a one-dimensional quantum walk with one defect, we can assume that, in (8), $r_+ = r_-$, $a_+ = a_-$ and so on. This implies that $\mu_3 = b_+ - b_- + c_+ - c_- = 0$. Setting $r_{\pm} = r_+$, $\nu_1 = \mu_1$ and $\nu_2 = \mu_2$ satisfies the first assertion. The necessary and sufficient condition for unitary equivalence follows from Theorem 2.8. \square

Clearly, Theorem 2.7 can be applied to complete two-phase quantum walks, though in this case, $U_{r, \mu}$ is not a complete two-phase quantum walk. Indeed, from the definition of complete two-phase quantum walks, we can assume that, in (8), $r_0 = r_+$, $a_0 = a_+$ and so on. Then, $\mu_1 = b_0 - b_- \neq 0$ in general, and the coefficients of $|e_1^{-1}\rangle\langle e_2^0|$ and $|e_1^{n-1}\rangle\langle e_2^n|$ ($n \geq 1$) of $U_{r, \mu}$ are not the same.

Hence, we provide the next theorem.

Theorem 2.12 *A complete two-phase quantum walk U is unitary equivalent to*

$$U_{r_+, r_-, \sigma_1, \sigma_2} = \sum_{n \geq 0} |e_1^{n-1}\rangle\langle r_+ e_1^n + s_+ e_2^n| + |e_2^{n+1}\rangle\langle -e^{i\sigma_1} s_+ e_1^n + e^{i\sigma_1} r_+ e_2^n| \\ + \sum_{n \leq -1} |e_1^{n-1}\rangle\langle r_- e_1^n + e^{i\sigma_2} s_- e_2^n| + |e_2^{n+1}\rangle\langle -s_- e_1^n + e^{i\sigma_2} r_- e_2^n|$$

for some $0 \leq r_+, r_- \leq 1$ and $\sigma_1, \sigma_2 \in \mathbb{R}$ with $s_{\varepsilon} = \sqrt{1 - r_{\varepsilon}^2}$ ($\varepsilon = +, -$). We write $U_{r_+, r_-, \sigma_1, \sigma_2} = U_{r, \sigma}$ for short. Moreover, when $0 < r_{\varepsilon}, r'_{\varepsilon} < 1$ and $\sigma_i, \sigma'_i \in [0, 2\pi)$, $U_{r, \sigma}$ and $U_{r', \sigma'}$ are unitary equivalent if and only if $r = r'$ and $\sigma = \sigma'$.

Proof. The proof is almost the same as that given for Theorems 2.7 and 2.8, but we present it here for completeness. Let

$$U = \sum_{n \in \mathbb{Z}} |\xi_{n-1, n}\rangle\langle \zeta_{n-1, n}| + |\xi_{n+1, n}\rangle\langle \zeta_{n+1, n}|$$

be a complete two-phase quantum walk. Then, by definition, Equation (2) can be written as

$$W_1 U W_1^* = \sum_{n \geq 0} |e_1^{n-1}\rangle\langle e^{ia_+} r_+ e_1^n + e^{ib_+} s_+ e_2^n| + |e_2^{n+1}\rangle\langle e^{ic_+} s_+ e_1^n + e^{id_+} r_+ e_2^n| \\ + \sum_{n \leq -1} |e_1^{n-1}\rangle\langle e^{ia_-} r_- e_1^n + e^{ib_-} s_- e_2^n| + |e_2^{n+1}\rangle\langle e^{ic_-} s_- e_1^n + e^{id_-} r_- e_2^n|$$

for some $0 \leq r_\varepsilon \leq 1$ and $a_\varepsilon, b_\varepsilon, c_\varepsilon, d_\varepsilon \in \mathbb{R}$ with $s_\varepsilon = \sqrt{1 - r_\varepsilon^2}$ ($\varepsilon = +, -$).

We then modify Step 2 as follows:

Step 2''. Let $\ell = (b_+ + c_- + \pi)/2$. Define $g_n, h_n \in \mathbb{R}$ by

$$g_n = \begin{cases} n(\ell - a_+) & (n \geq 0) \\ n(\ell - a_-) - a_- + a_+ & (n \leq -1) \end{cases}$$

and

$$h_n = \begin{cases} (n-1)(\ell - a_+) - b_+ + \ell & (n \geq 1) \\ (n-1)(\ell - a_-) + c_- + a_+ - a_- - \ell + \pi & (n \leq 0) \end{cases},$$

and a unitary W_2 on \mathcal{H} by

$$W_2 = \bigoplus_{n \in \mathbb{Z}} e^{ig_n} |e_1^n\rangle \langle e_1^n| + e^{ih_n} |e_2^n\rangle \langle e_2^n|.$$

Then, using $a_\varepsilon + d_\varepsilon + \pi = b_\varepsilon + c_\varepsilon$,

$$\begin{aligned} & e^{i\ell} W_2 W_1 U W_1^* W_2^* \\ &= \sum_{n \geq 0} |e_1^{n-1}\rangle \langle e^{i(a_+ - g_{n-1} + g_n - \ell)} r_+ e_1^n + e^{i(b_+ - g_{n-1} + h_n - \ell)} s_+ e_2^n| \\ & \quad + |e_2^{n+1}\rangle \langle e^{i(c_+ - h_{n+1} + g_n - \ell)} s_+ e_1^n + e^{i(d_+ - h_{n+1} + h_n - \ell)} r_+ e_2^n| \\ &+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle e^{i(a_- - g_{n-1} + g_n - \ell)} r_- e_1^n + e^{i(b_- - g_{n-1} + h_n - \ell)} s_- e_2^n| \\ & \quad + |e_2^{n+1}\rangle \langle e^{i(c_- - h_{n+1} + g_n - \ell)} s_- e_1^n + e^{i(d_- - h_{n+1} + h_n - \ell)} r_- e_2^n| \\ &= \sum_{n \geq 0} |e_1^{n-1}\rangle \langle r_+ e_1^n + s_+ e_2^n| + |e_2^{n+1}\rangle \langle -e^{i(c_+ - c_-)} s_+ e_1^n + e^{i(c_+ - c_-)} r_+ e_2^n| \\ &+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle r_- e_1^n + e^{i(b_- - b_+)} s_- e_2^n| + |e_2^{n+1}\rangle \langle -s_- e_1^n + e^{i(b_- - b_+)} r_- e_2^n| \\ &= \sum_{n \geq 0} |e_1^{n-1}\rangle \langle r_+ e_1^n + s_+ e_2^n| + |e_2^{n+1}\rangle \langle -e^{i\sigma_1} s_+ e_1^n + e^{i\sigma_1} r_+ e_2^n| \\ &+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle r_- e_1^n + e^{i\sigma_2} s_- e_2^n| + |e_2^{n+1}\rangle \langle -s_- e_1^n + e^{i\sigma_2} r_- e_2^n| \\ &= U_{r, \sigma}, \end{aligned}$$

where $\sigma_1 = c_+ - c_-$ and $\sigma_2 = b_- - b_+$. This shows the first assertion of this theorem.

Next, assume that $U_{r, \sigma}$ and $U_{r', \sigma'}$ are unitary equivalent, where $0 < r_\varepsilon, r'_\varepsilon < 1$ and $\sigma_i, \sigma'_i \in [0, 2\pi)$. Then, there exist $\lambda \in \mathbb{R}$ and a unitary operator $W = \bigoplus_{n \in \mathbb{Z}} W_n$ on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$ such that

$$e^{i\lambda} W U_{r, \sigma} W^* = U_{r', \sigma'}.$$

Here,

$$\begin{aligned} & e^{i\lambda} W U_{r, \sigma} W^* \\ &= e^{i\lambda} \sum_{n \geq 0} |W e_1^{n-1}\rangle \langle r_+ W e_1^n + s_+ W e_2^n| + |W e_2^{n+1}\rangle \langle -e^{i\sigma_1} s_+ W e_1^n + e^{i\sigma_1} r_+ W e_2^n| \\ &+ \sum_{n \leq -1} |W e_1^{n-1}\rangle \langle r_- W e_1^n + e^{i\sigma_2} s_- W e_2^n| + |W e_2^{n+1}\rangle \langle -s_- W e_1^n + e^{i\sigma_2} r_- W e_2^n| \end{aligned}$$

and

$$\begin{aligned} U_{r',\sigma'} &= \sum_{n \geq 0} |e_1^{n-1}\rangle \langle r'_+ e_1^n + s'_+ e_2^n| + |e_2^{n+1}\rangle \langle -e^{i\sigma'_1} s'_+ e_1^n + e^{i\sigma'_1} r'_+ e_2^n| \\ &+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle r'_- e_1^n + e^{i\sigma'_2} s'_- e_2^n| + |e_2^{n+1}\rangle \langle -s'_- e_1^n + e^{i\sigma'_2} r'_- e_2^n|. \end{aligned}$$

Considering $P_{n\pm 1} e^{i\lambda} W U_{r,\sigma} W^* P_n = P_{n\pm 1} U_{r',\sigma'} P_n$ for any $n \in \mathbb{Z}$, we have $W e_1^n = e^{iu_n} e_1^n$ and $W e_2^n = e^{iv_n} e_2^n$ for some $u_n, v_n \in \mathbb{R}$. Then,

$$\begin{aligned} &e^{i\lambda} W U_{r,\sigma} W^* \\ &= \sum_{n \geq 0} |e_1^{n-1}\rangle \langle e^{i(-u_{n-1}+u_n-\lambda)} r_+ e_1^n + e^{i(-u_{n-1}+v_n-\lambda)} s_+ e_2^n| \\ &\quad + |e_2^{n+1}\rangle \langle -e^{i(-v_{n+1}+u_n-\lambda+\sigma_1)} s_+ e_1^n + e^{i(-v_{n+1}+v_n-\lambda+\sigma_1)} r_+ e_2^n| \\ &+ \sum_{n \leq -1} |e_1^{n-1}\rangle \langle e^{i(-u_{n-1}+u_n-\lambda)} r_- e_1^n + e^{i(-u_{n-1}+v_n-\lambda+\sigma_2)} s_- e_2^n| \\ &\quad + |e_2^{n+1}\rangle \langle -e^{i(-v_{n+1}+u_n-\lambda)} s_- e_1^n + e^{i(-v_{n+1}+v_n-\lambda+\sigma_2)} r_- e_2^n|. \end{aligned}$$

Since $e^{i\lambda} W U_{r,\sigma} W^* = U_{r',\sigma'}$, we obtain $r = r'$. Moreover, comparing the coefficients of $|e_1^{n-1}\rangle \langle e_1^n|$, $|e_1^{n-1}\rangle \langle e_2^n|$ and $|e_2^{n+1}\rangle \langle e_1^n|$ yields

$$-u_{n-1} + u_n - \lambda = 0, \quad -u_{n-1} + v_n - \lambda = 0 \ (n \geq 0), \quad -v_{n+1} + u_n - \lambda = 0 \ (n \leq -1).$$

Here, we can assume that $u_0 = 0$, because $W U W^* = (e^{iw} W) U (e^{iw} W)^*$ for any $w \in \mathbb{R}$. Therefore, $u_n = n\lambda$, and this implies $v_n = u_{n-1} + \lambda = n\lambda$ ($n \geq 0$) and $v_{n+1} = u_n - \lambda = (n-1)\lambda$ ($n \leq -1$). Hence, $v_0 = 0$ and $v_0 = -2\lambda$ with the result that $\lambda = 0$ or π . Then, $-v_{n+1} + u_n - \lambda = 0$ for all $n \in \mathbb{Z}$, and therefore, $\sigma = \sigma'$, comparing the coefficients of $|e_2^{n+1}\rangle \langle e_2^n|$. This completes the proof. \square

From the above proof, if $e^{i\lambda} W U_{r,\sigma} W^* = U_{r,\sigma}$, then $\lambda = 0$ or π . When $\lambda = 0$, $v_n = u_n = 0$ and $W = I_{\mathcal{H}}$. When $\lambda = \pi$, $v_n = u_n = n\pi$ and $W = \bigoplus_{n \in \mathbb{Z}} (-1)^n I_{\mathcal{H}_n}$. Hence, we have the next corollary.

Corollary 2.13 *Let $0 < r_\varepsilon < 1$ ($\varepsilon = +, -$) and $\sigma_i \in [0, 2\pi)$ ($i = 1, 2$), and let $W = \bigoplus_{n \in \mathbb{Z}} W_n$ be a unitary on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$. Then, for $\lambda \in [0, 2\pi)$,*

$$e^{i\lambda} W U_{r,\sigma} W^* = U_{r,\sigma}$$

if and only if $\lambda = 0$ and $W = I_{\mathcal{H}}$ or $\lambda = \pi$ and $W = \bigoplus_{n \in \mathbb{Z}} (-1)^n I_{\mathcal{H}_n}$.

3 Unitary equivalent classes of one-dimensional quantum walks with initial states

In this section, we consider one-dimensional quantum walks with initial states. We assume that an initial state Φ is in \mathcal{H}_0 .

Definition 3.1 *One-dimensional quantum walks with initial states (U, Φ) and (U', Φ') are unitary equivalent if there exists a unitary $W = \bigoplus_{n \in \mathbb{Z}} W_n$ on $\mathcal{H} = \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_n$ such that*

$$U' = W U W^* \quad \text{and} \quad \Phi' = W \Phi.$$

Unitary equivalent classes of two-phase quantum walks with one defect with initial states are described as follows:

Theorem 3.2 *A two-phase quantum walk with one defect with an initial state (U, Φ) is unitary equivalent to $(U_{r,\mu}, \Phi_{\alpha,\theta})$ for some $0 \leq r_\varepsilon, \alpha \leq 1$ ($\varepsilon = +, -, 0$), $\mu_i, \theta \in \mathbb{R}$ ($i = 1, 2, 3$), where $\Phi_{\alpha,\theta} = \alpha e_1^0 + e^{i\theta} \sqrt{1 - \alpha^2} e_2^0$.*

Moreover, $(U_{r,\mu}, \Phi_{\alpha,\theta})$ and $(U_{r',\mu'}, \Phi_{\alpha',\theta'})$ with $0 < r_\varepsilon, r'_\varepsilon, \alpha, \alpha' < 1$ and $\mu_i, \mu'_i, \theta, \theta' \in [0, 2\pi)$ are unitary equivalent if and only if $r = r', \mu = \mu', \alpha = \alpha'$ and $\theta = \theta'$.

Proof. It was proved that U is unitary equivalent to $U_{r,\mu}$ for some r and μ in Theorem 2.7. Hence, there exists a unitary $W = \bigoplus_{n \in \mathbb{Z}} W_n$ on \mathcal{H} such that $WUW^* = U_{r,\mu}$. The state $W\Phi \in \mathcal{H}_0 = \mathbb{C}^2$ can be written as $W\Phi = \alpha e_1^0 + \beta e_2^0$ for some $\alpha, \beta \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 = 1$. Since $W\Phi$ and $e^{i\lambda}W\Phi$ are identified, we can assume that $0 \leq \alpha \leq 1$. Then, $\beta = e^{i\theta} \sqrt{1 - \alpha^2}$ for some $\theta \in \mathbb{R}$. Therefore, $W\Phi = \Phi_{\alpha,\theta}$ holds, and hence, (U, Φ) is unitary equivalent to $(U_{r,\mu}, \Phi_{\alpha,\theta})$.

Next, assume that $(U_{r,\mu}, \Phi_{\alpha,\theta})$ and $(U_{r',\mu'}, \Phi_{\alpha',\theta'})$ with $0 < r_\varepsilon, r'_\varepsilon, \alpha, \alpha' < 1$ and $\mu_i, \mu'_i, \theta, \theta' \in [0, 2\pi)$ are unitary equivalent. Then, by Theorem 2.8, $r = r'$ and $\mu = \mu'$. Moreover, if there exist $\lambda \in \mathbb{R}$ and a unitary operator $W = \bigoplus_{n \in \mathbb{Z}} W_n$ on \mathcal{H} such that

$$e^{i\lambda} W U_{r,\mu} W^* = U_{r,\mu},$$

then, by Corollary 2.9, $\lambda = 0$ and $W = I$ or $\lambda = \pi$ and $W = \bigoplus_{n \in \mathbb{Z}} (-1)^n I_{\mathcal{H}_n}$. Therefore, $W\Phi_{\alpha,\theta} = \Phi_{\alpha',\theta'}$ implies $\alpha = \alpha'$ and $\theta = \theta'$. \square

As a corollaries, and from Corollaries 2.10 and 2.11, we have the following.

Corollary 3.3 *A translation-invariant quantum walk (U, Φ) is unitary equivalent to $(U_r, \Phi_{\alpha,\theta})$ for some $0 \leq r, \alpha \leq 1$ and $\theta \in \mathbb{R}$.*

Moreover, $(U_r, \Phi_{\alpha,\theta})$ and $(U_{r'}, \Phi_{\alpha',\theta'})$ with $0 < r, r', \alpha, \alpha' < 1$ and $\theta, \theta' \in [0, 2\pi)$ are unitary equivalent if and only if $r = r', \alpha = \alpha'$ and $\theta = \theta'$.

Corollary 3.4 *A one-dimensional quantum walk with one defect (U, Φ) is unitary equivalent to $(U_{r,\nu}, \Phi_{\alpha,\theta})$ for some $0 \leq r_\varepsilon, \alpha \leq 1$ ($\varepsilon = \pm, 0$) and $\nu_i, \theta \in \mathbb{R}$ ($i = 1, 2$).*

Moreover, $(U_{r,\nu}, \Phi_{\alpha,\theta})$ and $(U_{r',\nu'}, \Phi_{\alpha',\theta'})$ with $0 < r_\varepsilon, r'_\varepsilon, \alpha, \alpha' < 1$ and $\nu_i, \nu'_i, \theta, \theta' \in [0, 2\pi)$ are unitary equivalent if and only if $r = r', \nu = \nu', \alpha = \alpha'$ and $\theta = \theta'$.

The proof of the next theorem is almost the same as that given for Theorem 3.2 and is omitted.

Theorem 3.5 *A complete two-phase quantum walk (U, Φ) is unitary equivalent to $(U_{r,\sigma}, \Phi_{\alpha,\theta})$ for some $0 \leq r_\varepsilon, \alpha \leq 1$ ($\varepsilon = +, -$) and $\sigma_i, \theta \in \mathbb{R}$ ($i = 1, 2$).*

Moreover, $(U_{r,\sigma}, \Phi_{\alpha,\theta})$ and $(U_{r',\sigma'}, \Phi_{\alpha',\theta'})$ with $0 < r_\varepsilon, r'_\varepsilon, \alpha, \alpha' < 1$ and $\sigma_i, \sigma'_i, \theta, \theta' \in [0, 2\pi)$ are unitary equivalent if and only if $r = r', \sigma = \sigma', \alpha = \alpha'$ and $\theta = \theta'$.

References

- [1] Aharanov, L., Davidovich, N., Zagury, N.: Quantum random walks, Phys. Rev. A **48**, 1687-1690 (1993)

- [2] Ambainis, A., Bach, E., Nayak, A., Vishwanath, A., Watrous, J.: One-dimensional quantum walks, Proc. 33th ACM Symposium of the Theory of Computing, 37-49 (2001)
- [3] Cantero, M. J., Grünbaum, F. A., Moral, L., Velázquez, L.: Matrix valued Szegő polynomials and quantum random walks, Commun. Pure Appl. Math. **58**, 464-507 (2010)
- [4] Cantero, M. J., Grünbaum, F. A., Moral, L., Velázquez, L.: One-dimensional quantum walks with one defect, Rev. Math. Phys. **24**, 1250002 (2012)
- [5] Cantero, M. J., Grünbaum, F. A., Moral, L., Velázquez, L.: The CGMV method for quantum walks, Quantum Inf. Process. **11**, 1149-1192 (2012)
- [6] Endo, S., Endo, T., Konno, N., Segawa, E., Takei, M.: Weak limit theorem of a two-phase quantum walk with one defect, arXiv:1412.4309.
- [7] Endo, S., Endo, T., Konno, N., Segawa, E., Takei, M.: Limit theorems of a two-phase quantum walk with one defect, Quantum Inf. Comput. **15**, 1373-1396 (2015)
- [8] Endo, S., Konno, N.: Weak convergence of the Wojcik model, Yokohama Math. J. **61**, 87-111 (2015)
- [9] Endo, S., Konno, N.: The stationary measure of a space-inhomogeneous quantum walk on the line, Yokohama Math. J. **60**, 33-47 (2014)
- [10] Endo, S., Konno, N., Segawa, E., Takei, M.: A one-dimensional Hadamard walk with one defect, Yokohama Math. J. **60**, 49-90 (2014)
- [11] Endo, T., Konno, N., Obuse, H.: Relation between two-phase quantum walks and the topological invariant, arXiv:1511.04230.
- [12] Goyal, S. K., Konrad, T., Diósi, L.: Unitary equivalence of quantum walks, Phys. Lett. A **379**, 100-104 (2015)
- [13] Gudder, S. P.: Quantum Probability, Academic Press, 1988.
- [14] Kitagawa, T., Rudner, M. S., Berg, E., Demler, E.: Exploring topological phases with quantum walks, Phys. Rev. A **82**, 033429 (2010)
- [15] Konno, N.: Quantum random walks in one dimensional, Quantum Inf. Process. **1**, 345-354 (2002)
- [16] Konno, N.: One-dimensional discrete-time quantum walks on random environment, Quantum Inf. Process. **8**, 387-399 (2009)
- [17] Konno, N.: Localization of an inhomogeneous discrete-time quantum walk on the line, Quantum Inf. Process. **9**, 405-418 (2010)
- [18] Konno, N., Łuczak, T., Segawa, E.: Limit measures of inhomogeneous discrete-time quantum walks in one dimensional, Quantum Inf. Process. **12**, 33-53 (2013)
- [19] Ohno, H.: Unitary equivalent classes of one-dimensional quantum walks, Quantum Inf. Process. **15**, 3599-3617 (2016)

- [20] Segawa, E., Suzuki, A.: Generator of an abstract quantum walk, *Quantum Stud. Math. Found.* **3**, 11-30 (2016)
- [21] Shikano, Y., Katsura, H.: Localization and fractality in inhomogeneous quantum walks with self-duality, *Phys. Rev. E* **82**, 031122 (2010)
- [22] Venegas-Andraca, S. E.: Quantum walks: a comprehensive review, *Quantum Inf. Process.* **11**, 1015-1106 (2012)
- [23] Wójcik, A., Łuczak, T., Kurzyński, P., Grudka, A., Gdala, T., Bednarska-Bzdega, M.: Trapping a particle of a quantum walk on the line, *Phys. Rev. A* **85**, 012329 (2012)